

Quantization and 2π Periodicity of the Axion Action in Topological Insulators

M.M. Vazifeh and M. Franz

Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, Canada V6T 1Z1

(Dated: November 11, 2010)

The Lagrangian describing the bulk electromagnetic response of a three-dimensional strong topological insulator contains a topological ‘axion’ term of the form $\theta \mathbf{E} \cdot \mathbf{B}$. It is often stated (without proof) that the corresponding action is quantized on periodic space-time and therefore invariant under $\theta \rightarrow \theta + 2\pi$. Here we provide a simple, physically motivated proof of the axion action quantization on the periodic space-time, assuming only that the vector potential is consistent with single-valuedness of the electron wavefunctions in the underlying insulator.

Introduction — Topological insulators are time-reversal (\mathcal{T}) invariant crystalline solids with insulating bulk band structure and topologically protected gapless surface states.^{1,2} These surface states are robust against the effects of non-magnetic disorder and form a theoretical basis for numerous exotic phenomena^{3–6} as well as proposed practical applications.^{7,8} Their presence has been detected in several materials with a strong spin-orbit interaction.^{9–13}

An alternative characterization of a strong topological insulator^{14–16} (STI) follows from its unusual response to applied electromagnetic fields which is encoded in a bulk ‘axion’ term^{4,17} of the form

$$\mathcal{L}_{\text{axion}} = \theta \left(\frac{e^2}{2\pi\hbar c} \right) \mathbf{B} \cdot \mathbf{E}, \quad (1)$$

with $\theta = \pi$. The axion term (1) appears in the electromagnetic Lagrangian in addition to the standard Maxwell term. Eq. (1) underlies the topological magnetoelectric effect^{4,17} in which electric (magnetic) polarization is induced by external magnetic (electric) field, as well as the Witten effect^{18,19} that attaches a fractional electric charge to a magnetic monopole.

The axion term (1) has been introduced in the context of high-energy physics decades before the discovery of STIs to resolve CP non-violation problem in quantum chromodynamics^{20–22} (QCD). The corresponding $\theta(\mathbf{x}, t)$ field is known to particle physicists as the axion field²³. The action of the uniform axion field can be viewed as a topological term for the θ vacuum in QCD arising from nontrivial topology of such a vacuum.

For a generic value of θ the axion term breaks \mathcal{T} as well as parity \mathcal{P} . This is because under time-reversal $\mathbf{B} \rightarrow -\mathbf{B}$, $\mathbf{E} \rightarrow \mathbf{E}$, while under spatial inversion $\mathbf{B} \rightarrow \mathbf{B}$, $\mathbf{E} \rightarrow -\mathbf{E}$. What allows the \mathcal{T} - and \mathcal{P} -invariant insulators to possess an axion term with $\theta = \pi$ is the 2π -periodicity of the axion action $S_{\text{axion}} = \int dt d^3x \mathcal{L}_{\text{axion}}$ in parameter θ . Specifically, on periodic space-time (that is used to model an infinite bulk crystal), the integral in the axion action is quantized,

$$\left(\frac{e^2}{2\pi\hbar c} \right) \int dt d^3x \mathbf{B} \cdot \mathbf{E} = N\hbar, \quad (2)$$

with N integer. All physical observables depend on $\exp(iS_{\text{axion}}/\hbar)$ and are thus invariant under a global

transformation $\theta \rightarrow \theta + 2\pi$. Consequently, $\theta = \pi$ and $\theta = -\pi$ are two equivalent points and describe a \mathcal{T} - and \mathcal{P} -invariant system. Conversely, in a system invariant under \mathcal{P} or \mathcal{T} the value of θ is quantized to 0 or π .

The statement regarding the quantization of the expression (2) on periodic space-times has been made in several influential papers^{4,6,17,23} but no simple physical explanation has been given of its validity. One way to understand the quantization is using mathematical theory of fibre bundles²⁴ in which the axion action is an integral of a second Chern character associated with an abelian gauge theory. In topology Chern characters are forms whose integral over closed base space returns integer values. Hence, once the base space is compact the topological axion action is necessarily quantized. A well-known example in the context of condensed matter physics is the transverse conductivity of a quantum Hall insulator which can be expressed as a first Chern integral over the BZ and hence it turns out to be strictly quantized.^{25,26}

Since the quantization of the axion term and the related θ -periodicity underlies the essential element of the theory of topological insulators it is important to have a clear physical understanding of its origin. In the rest of this paper we provide a direct and simple proof of the axion action quantization on periodic space-time. We also consider a non-periodic case where the axion action remains quantized. Our proof is based on the electromagnetic field decomposition into an ‘externally imposed’ uniform constant part which we show can have non-zero contribution to S_{axion} and a part generated by space-time periodic charge and current configurations whose contribution vanishes. The quantization condition (2) follows from the requirement that the underlying vector potential be consistent with the single-valuedness of the electron wave-functions.²⁷ In our proof we assume that no magnetic monopoles are present but in closing we comment on the situation with monopoles. As a byproduct of our proof we find that for abelian gauge field the invariant based on the second Chern character is fully determined by first Chern characters associated with orthogonal coordinate planes in four-dimensional space-time. In this way abelian case is different from the better known non-abelian case²⁴ where due to the presence of instantons the second Chern number can be non-zero even if all first Chern numbers vanish.

General considerations — In a covariant formulation

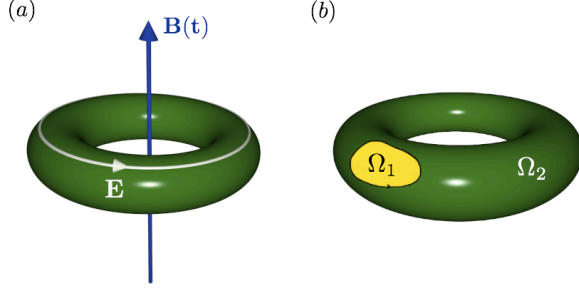


FIG. 1: (Color online) (a) A magnetic field increasing linearly with time and confined to a torus hole produces a uniform and constant electric field along the torus. (b) A closed path on the torus can be thought of as enclosing two areas, Ω_1 and Ω_2 .

with the speed of light $c = 1$ the axion action can be written as²³

$$\frac{1}{\hbar} S_{\text{axion}} = \frac{\theta}{8\Phi_0^2} \int d^4x \varepsilon^{\mu\nu\alpha\beta} F_{\mu\nu}(x) F_{\alpha\beta}(x) \quad (3)$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the electromagnetic field tensor and $\Phi_0 = h/e$ is the quantum of magnetic flux. In the following we consider a space-time hypercube of side L with periodic boundary conditions imposed on $F_{\mu\nu}(x)$ in all directions.

In the absence of monopoles integration by parts gives

$$\frac{1}{\hbar} S_{\text{axion}} = \frac{\theta}{4\Phi_0^2} \int d^4x \varepsilon^{\mu\nu\alpha\beta} \partial_\alpha [F_{\mu\nu}(x) A_\beta(x)] \quad (4)$$

At first glance, from the periodicity of space and time one might conclude that the integral in (4) vanishes for a general electromagnetic field tensor since it can be written as a three dimensional hyper-surface integral of $F_{\mu\nu} A_\beta$ which is zero if this function is periodic in space-time coordinates. However, a simple example of constant uniform fields $\mathbf{E} \parallel \mathbf{B}$ shows this conclusion to be erroneous. The point is that in general the gauge field 4-vector of a periodic electromagnetic field is not periodic in space and time. As an example consider a lower dimensional case of T^2 torus with a magnetic flux through its hole increasing linearly with time (Fig. 1a). This induces an electric field on the torus which is constant and therefore periodic in time and the coordinates that parametrize the torus. However the line integral of the gauge field over the non-contractible loop enclosing the magnetic flux is nonzero which means that the gauge field cannot be chosen periodic. For the field configurations of this type, containing field lines along non-contractible loops, S_{axion} will be non-vanishing and we must consider these with special care.

A question arises here: in general for what kind of periodic electromagnetic field configurations in 3 spatial dimensions the gauge field cannot be chosen periodic? A

gauge potential A_μ cannot be chosen periodic if

$$\oint_{\square} d\ell \cdot A \neq 0 \quad (5)$$

where the line integral is over any $L \times L$ square located in one of the coordinate planes $x_\mu x_\nu$ with $\mu \neq \nu$ on the hyper-cube. We note that the above integral (5) is gauge invariant and, due to the periodicity of $F_{\mu\nu}(x)$, its value is independent of the position of the $L \times L$ square, i.e. it is invariant under any space-time translation. In terms of the field tensor Eq. (5) can be written as

$$\int_{\square} dx_\mu dx_\nu F_{\mu\nu} \neq 0, \quad (6)$$

with no summation over μ, ν . Physically, this means that total magnetic flux through one of the spatial faces of the hypercube is non-zero and a similar condition for the electric field (see below).

The above considerations motivate a decomposition of the gauge potential into two pieces,

$$A_\mu(x) = A_\mu^0(x) + \delta A_\mu(x), \quad (7)$$

such that

$$\oint_{\square} d\ell \cdot \delta A = 0. \quad (8)$$

Hence δA_μ can be chosen periodic, while $A_\mu^0(x)$ contains any non-periodic part. Similarly, we write

$$F_{\mu\nu}(x) = F_{\mu\nu}^0(x) + \delta F_{\mu\nu}(x), \quad (9)$$

with $F_{\mu\nu}^0 \equiv \partial_\mu A_\nu^0 - \partial_\nu A_\mu^0$. To make this decomposition unique (up to a gauge transformation) we furthermore impose a condition that components of $F_{\mu\nu}^0$ are uniform and constant,

$$F_{\mu\nu}^0 = \frac{1}{L^2} \int_{\square} dx_\mu dx_\nu F_{\mu\nu}. \quad (10)$$

In terms of electric and magnetic field vectors our decomposition corresponds to

$$\mathbf{E} = \mathbf{E}_0 + \delta \mathbf{E}, \quad \mathbf{B} = \mathbf{B}_0 + \delta \mathbf{B} \quad (11)$$

where $\mathbf{E}_0, \mathbf{B}_0$ are constant uniform fields while $\delta \mathbf{E}, \delta \mathbf{B}$ are space-time varying fields derived from the periodic gauge potential $\delta A_\mu(x)$. The constant fields can only be produced by magnetic and electric fluxes through the holes in the T^3 torus embedded in a four dimensional space and it is not possible to devise non-singular charge and current sources within the periodic three dimensional space to produce them.²⁸

Fields $\delta \mathbf{E}$ and $\delta \mathbf{B}$ are produced by ordinary charge and current sources. They have the following physical properties: (i) Magnetic fluxes associated with these magnetic fields through each spatial face vanish,

$$\varepsilon^{ijk} \int_{\square} dx_i dx_j \delta B_k = 0 \quad i, j, k = 1, 2, 3. \quad (12)$$

There is no summation on indices and the equation holds for all x_k and x_0 . (ii) The integral over any space-time face

$$\int_{\square} dx_0 dx_i \delta E_i = 0, \quad (13)$$

with no summation on $i = 1, 2, 3$. (i) and (ii) are properties of the fields produced by a general space-time periodic charge and current sources.

Action evaluation — With this preparation we can now proceed to evaluate the axion action. It is most convenient to employ Eq. (4) where in view of our decomposition (8,9) the expression $F_{\mu\nu}A_\beta$ is replaced by

$$F_{\mu\nu}^0 A_\beta^0 + 2F_{\mu\nu}^0 \delta A_\beta + \delta F_{\mu\nu} \delta A_\beta. \quad (14)$$

An integration by parts has been performed on $\delta F_{\mu\nu} A_\beta^0$ to obtain the factor of 2 in the middle term. Now the second and the third term in the above expression (14) are explicitly space-time *periodic* and therefore their contribution to S_{axion} identically vanishes. The only contribution to the action comes from the first term which represents the uniform constant part of the electromagnetic fields. Thus,

$$\frac{1}{\hbar} S_{\text{axion}} = \frac{\theta}{\Phi_0^2} \int d^4x \mathbf{E}_0 \cdot \mathbf{B}_0. \quad (15)$$

It remains to be demonstrated that the action is quantized for these constant and uniform fields.

Our arguments thus far have been purely classical. At the level of classical electrodynamics, clearly, the integral in Eq. (15) can attain any desired value and is not quantized. To proceed, we must recall that in the present context the axion term results from integrating out the electron degrees of freedom in a topological insulator. Electron behavior is inherently quantum mechanical. The axion action quantization then follows from the requirement that the gauge potential A_μ that couples to the electron wavefunctions be consistent with the quantum theory of electrons in periodic space-time.

In the following we assume for simplicity that our fields are pointed along the x_3 direction, $\mathbf{E}_0 = E_3 \hat{x}_3$ and $\mathbf{B}_0 = B_3 \hat{x}_3$. Other components can be treated in an identical fashion. For this configuration we may decompose our space-time torus T^4 into a direct product $T_{12}^2 \times T_{03}^2$ and write

$$\frac{1}{\hbar} S_{\text{axion}} = \frac{\theta}{\Phi_0^2} \int_{\square} dx_1 dx_2 B_3 \int_{\square} dx_0 dx_3 E_3. \quad (16)$$

It remains to show that each of these integrals is an integer multiple of magnetic flux quantum Φ_0 . The first integral represents the total magnetic flux through the $x_1 x_2$ face of the hypercube. The quantization of this term follows from the standard arguments for the electron motion in applied magnetic field, which we now briefly review for completeness.

Imagine an arbitrary closed path \mathcal{C} on the T_{12}^2 torus. As illustrated in Fig. 1b it encloses area denoted as Ω_1 .

Alternately, it can be viewed as enclosing its complement on T_{12}^2 denoted as Ω_2 . Using Stoke's theorem we may write

$$\int_{\Omega_1} \mathbf{B} \cdot d\mathbf{S} = \oint_{\mathcal{C}} \mathbf{A} \cdot d\mathbf{l} \quad (17)$$

$$\int_{\Omega_2} \mathbf{B} \cdot d\mathbf{S} = - \oint_{\mathcal{C}} \mathbf{A}' \cdot d\mathbf{l} \quad (18)$$

where the prime on the vector potential signifies the subtle but important fact that the equality is required to hold only up to a gauge transformation $A_\mu \rightarrow A'_\mu = A_\mu - \partial_\mu f$, with $f(x)$ a scalar function. Now the line integral of \mathbf{A} along a closed path is normally thought of as a gauge invariant quantity in which case adding Eqs. (17) and (18) immediately implies $\int_{\Omega_1 + \Omega_2} \mathbf{B} \cdot d\mathbf{S} = 0$. This suggests that S_{axion}/\hbar is indeed quantized but the only value allowed is 0. However, there exists a class of ‘large’ gauge transformations $f(x)$ which change the value of the line integral but leave the wavefunction single valued. The latter transforms as $\Psi(x) \rightarrow \Psi'(x) = e^{ief(x)}\Psi(x)$ and the relevant $f(x)$ contains a vortex (a Dirac string) at some point of the T_{12}^2 torus, i.e. $e^{ief(x)} \sim e^{ien\varphi}$ where φ is an angle in $x_1 x_2$ plane measured from the vortex center and n is an integer. Since $\oint_{\mathcal{C}} \nabla f \cdot d\mathbf{l} = 2\pi n$ the inclusion of large gauge transformations of this type can be seen from Eqs. (17) and (18) to allow for non-zero quantized values $\int_{\square} dx_1 dx_2 B_3 = n\Phi_0$.

One can advance the same argument to establish the quantization of the second surface integral in Eq. (16). Consider a closed path, this time on T_{03}^2 , enclosing Ω_1 and Ω_2 regions. It is straightforward to check that all steps proceed exactly as before. The large gauge transformations now involve space-time vortices in $f(x)$ (i.e. vortices in the $x_0 x_3$ plane) and lead to analogous result $\int_{\square} dx_0 dx_3 E_3 = m\Phi_0$ with m integer.

Combining the above results we find

$$\frac{1}{\hbar} S_{\text{axion}} = N\theta, \quad (19)$$

with $N = nm$. Eq. (19) shows that the axion action for electromagnetic field is quantized on periodic space-time and, consequently, the amplitude $\exp(iS_{\text{axion}}/\hbar)$ is invariant under the shift of the axion angle θ by any integer multiple of 2π .

A more abstract and rigorous way to think of the quantization of these quantities is using fibre bundle mathematics mentioned briefly in the beginning. The fibre bundles²⁴ can be classified in terms of the so called Chern characters. These are forms whose integral over closed base space of the bundle always return an integer number. One consequence is that the integral of a first Chern character of the Abelian $U(1)$ gauge theory, $F_{\mu\nu}/\Phi_0$ on the closed base space $T_{\mu\nu}^2$ must always be an integer. On the other hand the axion action is a second Chern character integral evaluated for this abelian gauge theory. We showed that this can be written as a product of two first Chern character integrals whose quantization, as we discussed, has a clear physical interpretation.

Non-periodic systems — Assuming periodic boundary conditions in all directions is the simplest way to avoid edges and to concentrate on the bulk response. However, in real experimental setup one must deal with a situation where the fields are present in a finite portion of space and over a finite time duration. The question arises whether the axion action remains quantized under these non-periodic conditions. The answer is “yes” provided that one additional condition on the gauge potential is satisfied. Specifically, it is possible to show that Eq. (2) remains valid if (i) the fields \mathbf{B} and \mathbf{E} vanish outside a space-time volume \mathcal{V} and (ii) the underlying gauge field A_μ is such that its presence cannot be detected by any Aharonov-Bohm type experiment performed using charge e particles outside \mathcal{V} . For the magnetic field this implies, for example, that the total flux enclosed by any closed trajectory is $n\Phi_0$ with n integer. In that case the Aharonov-Bohm phase acquired by charge e particle is $2\pi n$ and thus indistinguishable from 0.

Inclusion of monopoles — In passing from Eq. (3) to (4) we assumed that a term $A_\beta \varepsilon^{\mu\nu\alpha\beta} \partial_\alpha F_{\mu\nu}$ that appears in the integration by parts vanishes on the account of partial derivatives commuting and $\varepsilon^{\mu\nu\alpha\beta}$ being antisymmetric. This assumption fails in the presence of magnetic monopoles. Consider *e.g.* the $\beta = 0$ component of the above expression which equals $2A_0 \nabla \cdot \mathbf{B}$. In the presence of the non-vanishing monopole density $\nabla \cdot \mathbf{B} \neq 0$ such term will give non-zero contribution to S_{axion} whenever A_0 is non-zero. Similarly, $\beta = 1, 2, 3$ terms correspond

to monopole currents and may be non-vanishing as well. Our proof of θ -periodicity given above must be modified in the presence of monopoles.

The simplest modification applies to the special case when there are no electrical charges or currents in the system and fields are sourced purely by magnetic charges and currents. In this case one can perform a duality transformation²⁸ which interchanges \mathbf{E} and \mathbf{B} and the proof proceeds exactly as before in terms of dual field variables. In the most general case when there are both electric and magnetic charges/currents present a form of θ -periodicity still holds but its statement and proof now involve several subtle points.²⁹ Specifically one must take special care when dealing with non-single valued vector potential and one must also take into account the Witten effect.¹⁸

Closing thoughts — We have presented a simple and intuitive proof of the quantization of the topological axion action on periodic space-time. Our considerations show that the theory is invariant under a global $\theta \rightarrow \theta + 2\pi$ transformation consistent with the \mathbb{Z}_2 character of the fundamental ‘strong’ invariant describing the physics of time-reversal invariant band insulators.

Acknowledgment — The authors benefited greatly from the discussions and correspondence with I. Affleck, H. Karimi, J.E. Moore, G. Rosenberg, G.E. Volovik, X.-L. Qi and G. Semenoff. Support for this work came from NSERC and CIFAR.

-
- ¹ J. E. Moore, Nature **464**, 194 (2010).
 - ² M.Z. Hasan, C.L. Kane, arXiv:1002.3895
 - ³ L. Fu and C. L. Kane, Phys. Rev. Lett. **100**, 096407 (2008).
 - ⁴ X.-L. Qi, T. Hughes, and S.-C. Zhang, Phys. Rev. B **78**, 195424 (2008).
 - ⁵ B. Seradjeh, J.E. Moore, and M. Franz, Phys. Rev. Lett. **103**, 066402 (2009).
 - ⁶ X. L. Qi, R. Li, J. Zang, S.-C. Zhang, Science **323**, 1184 (2009).
 - ⁷ T. Yokoyama, Y. Tanaka, and N. Nagaosa, Phys. Rev. B **81**, 121401(R) (2010).
 - ⁸ I. Garate and M. Franz, Phys. Rev. Lett. **104**, 146802 (2010).
 - ⁹ M. Konig *et al.*, Science **318**, 766 (2007)
 - ¹⁰ D. Hsieh *et al.*, Nature **452**, 970 (2008).
 - ¹¹ Y. Xia *et al.*, Nature Phys. **5**, 398 (2009).
 - ¹² Chen, Y.L. *et al.* Science **325**, 178181 (2009).
 - ¹³ D. Hsieh *et al.*, Science **323**, 919 (2009).
 - ¹⁴ L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. **98**, 106803 (2007).
 - ¹⁵ J. E. Moore and L. Balents, Phys. Rev. B **75**, 121306(R) (2007).
 - ¹⁶ R. Roy, Phys. Rev. B **79**, 195322 (2009).
 - ¹⁷ A.M. Essin, J.E. Moore, D. Vanderbilt, Phys. Rev. Lett. **102**, 146805 (2009).
 - ¹⁸ E. Witten, Phys. Lett. B **86**, 283 (1979).
 - ¹⁹ G. Rosenberg and M. Franz, arXiv:1001.3179.
 - ²⁰ R. D. Peccei and H. R. Quinn, Phys. Rev. Lett. **38**, 1440 (1977).
 - ²¹ S. Weinberg, Phys. Rev. Lett. **40**, 223 (1978).
 - ²² F. Wilczek, Phys. Rev. Lett. **40**, 279 (1978).
 - ²³ F. Wilczek, Phys. Rev. Lett. **58**, 1799 (1987).
 - ²⁴ M. Nakahara, Geometry, Topology and Physics (Adam Hilger, Bristol, 1990).
 - ²⁵ D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).
 - ²⁶ J. E. Avron, R. Seiler and B. Simon, Phys. Rev. Lett. **51**, 51 (1983).
 - ²⁷ Y. Aharonov and D. Bohm, Phys. Rev. **115**, 485 (1959).
 - ²⁸ J.D. Jackson, *Classical Electrodynamics* (3rd Edition, Wiley, 1998).
 - ²⁹ M.M. Vazifteh (unpublished).